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LETTER TO THE EDITOR

Commutation relations for periodic operators

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Abstract. Although periodic variables are common in quantum systems, there is still some question of their proper commutation relations. We show that the standard commutation relations, when applied carefully, do not lead to inconsistencies. We discuss other approaches to the problem in the literature.

A variety of quantum systems are described by wavefunctions that are strictly periodic in some generalized phase variable. Most fundamental, perhaps, is the azimuthal angle, $\hat{\theta}$, of an electron in its orbital, whose conjugate operator $\hat{L}_z$ measures the z-component of the angular momentum. Since we require the wavefunction to satisfy periodic boundary conditions, so that $\Psi(\theta=0)=\Psi(\theta=2\pi)$, with $0\leqslant\theta\leqslant 2\pi$, we refer to θ as being *compact* (defined only over a finite interval) and to $\Psi(\theta)$ as *periodic*. Another example is the phase operator $\hat{\phi}$, which measures the phase difference of the pair wavefunction across a Josephson junction [1–6]. If the junction is made from two disjoint superconductors (i.e. not from a ring of superconductors) then physical states in which ϕ differs by multiples of 2π are indistinguishable and we again have to choose periodic boundary conditions. A third example of recent importance is a small normal metal ring [7–10]. If we consider the simple case of a single electron confined to a mesoscopic normal metal ring, then its description again requires a compact variable, Θ, that denotes the angular position of an electron on the ring, and again we require the single-valuedness boundary condition $\Psi(\Theta=0)=\Psi(\Theta=2\pi)$. To maintain this periodic boundary condition in the presence of an external magnetic flux the electron will adjust its momentum, thereby generating a net current. A related phenomenon due to the single-valuedness of the wavefunction leads to the Aharonov–Bohm effect [11]. Other examples of phase variables occur in optics, atomic physics, and many solid state systems.

It is then surprising that there is some question as to the proper commutation relations for phase operators [12–17]. For the sake of concreteness, we consider the case of $\hat{L}$, the angular momentum operator, and $\hat{\theta}$, the angular position operator of a particle confined to a one-dimensional ring of radius R, such as a bead on a circular loop. This system is described by smooth, square integrable wavefunctions on the interval $[0, 2\pi]$ that obey periodic boundary conditions in θ. This example is distinct

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from cases where the 'momentum' takes on only non-negative integral values [14]. Given the standard Schrödinger representation for the angular momentum operator, $\hat{L}=-\mathrm{i}\hbar\partial/\partial\theta$, it immediately follows that the commutation relation is

$$[\hat{L},\hat{\theta}]=-\mathrm{i}\hbar. \tag{1}$$

However, if we take matrix elements in the angular momentum basis, $|m\rangle$, where $\hat{L}|m\rangle=\hbar m|m\rangle$, we find

$$\langle m|[\hat{L},\hat{\theta}]|n\rangle=\langle m|\hat{L}\hat{\theta}-\hat{\theta}\hat{L}|n\rangle=(m-n)\langle m|\hat{\theta}|n\rangle \tag{2}$$

where we have invoked the self-adjointness of $\hat{L}$. Equating this to the matrix element of the right-hand side of (1), we obtain the contradictory result

$$(m-n)\langle m|\hat{\theta}|n\rangle=-\mathrm{i}\hbar\delta_{mn}. \tag{3}$$

If $m=n$, the right-hand side is non-zero, while the left-hand side is zero [12, 17].

It has been argued [12-17] that this paradox is due to the fact that $\hat{\theta}$ is not an allowable operator on the space of periodic functions, unless one defines the phase operator in such a way that it is itself periodic. Note that the derivation of (1) using the standard definition of $\hat{L}$ and $\hat{\theta}$ is not claimed to be wrong, but rather that the use of $\hat{\theta}$ itself is inconsistent, because equally valid arguments lead to contradictory results. It is the aim of this letter to resolve this paradox, by showing that (3) is based on incorrect mathematical transformations. After doing so we will briefly mention other approaches to this problem.

First, we note that it is indeed true that $\hat{\theta}$ by itself *alone* is not an allowable operator on the space of periodic functions (that do not vanish on the boundaries), since it projects them out of the original 'Hilbert space'†. Nevertheless, this argument does not prove that appropriate functions of $\hat{\theta}$, or combinations of $\hat{\theta}$ and $\hat{L}$ are forbidden. Consider the operator $\mathrm{e}^{\mathrm{i}\hat{\theta}}$, which is manifestly periodic; if we expand it in $\hat{\theta}$, each term of the sum is not. Only after we recombine all the terms of an expansion that we can determine whether or not the original operator is periodic. A second example is the angular velocity of the particle moving on the ring. Here physics dictates that the velocity operator $\dot{\hat{\theta}}$ is a periodic operator. Mathematically, this is clear from its definition

$$\mathrm{i}\hbar\dot{\hat{\theta}}=[\hat{\theta},H] \tag{4}$$

which shows that $\dot{\hat{\theta}}$ is invariant under the transformation $\hat{\theta}\to\hat{\theta}+2\pi$, provided that H is periodic in $\hat{\theta}$. A third example is the commutator itself, $C(\hat{\theta})\equiv[\hat{L},\hat{\theta}]$ which is periodic for the same reason as $\dot{\hat{\theta}}$. We see that the mere presence of the operator $\hat{\theta}$ does not immediately imply that a given expression is impermissible in our subspace of periodic functions.

Second, one must recognize that the Dirac notation of (2) is ambiguous and thus can be misleading. To avoid this ambiguity we introduce the following inner product notation, in an angular momentum basis,

$$(m,\hat{\mathscr{A}}n)\equiv\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\theta\,\mathrm{e}^{-\mathrm{i}m\theta}\,\hat{\mathscr{A}}\,\mathrm{e}^{\mathrm{i}n\theta} \tag{5}$$

where $\hat{\mathscr{A}}$ is an arbitrary operator.

† To be more precise, it projects periodic wavefunctions out of the definition range of the self-adjoint operator $\hat{L}$, a range which is a dense subset of the full Hilbert space of square integrable functions. For a discussion of such issues see [19].

The difficulty comes in taking the adjoint of $\hat{L}$. In the Dirac notation we have used

$$\langle m|\hat{L}\hat{\theta}|n\rangle = m\langle m|\hat{\theta}|n\rangle \qquad \text{(wrong)} \tag{6}$$

which is not correct because $\hat{L}$ is not self-adjoint on $\hat{\theta}|n\rangle$ (because $\hat{\theta}|n\rangle$ is not a periodic ket). This was noted by Carruthers and Nieto [16] who then went on to conclude that $\hat{\theta}$ is not an allowable operator and should be replaced by a periodic extension, to be discussed below. However, for reasons given earlier, it is not appropriate to consider only one term in the commutator and judge the whole expression as meaningless [18]. Thus, we proceed to evaluate this term using the inner product notation carefully

$$(m, \hat{L}\hat{\theta}n) = (\hat{L}m, \hat{\theta}n) - \mathrm{i}\hbar \tag{7}$$

where the term $-\mathrm{i}\hbar$ comes from the boundary term in the partial integration. Using this result in evaluating the *full* commutator we have

$$(m, \{\hat{L}\hat{\theta} - \hat{\theta}\hat{L}\}n) = \hbar(m-n)(m, \hat{\theta}n) - \mathrm{i}\hbar = -\mathrm{i}\hbar\delta_{mn} \tag{8}$$

which is in complete agreement with (1) and thus resolves our paradox.

The matrix elements of the terms $\hat{L}\hat{\theta}$ and $\hat{\theta}\hat{L}$ are always calculable and finite and thus mathematically well defined. Each term by itself is not an allowable operator on our space of periodic wavefunctions, in particular in the sense that we have to be careful when using the standard operator manipulations as is clear from (6) and (7). However, this does not preclude the occurrence of these terms in intermediate steps of the calculation. What matters in this context is that their difference *is* an allowable operator. In using the Dirac notation on periodic systems, the self-adjointness of an operator must be used with care whenever non-periodic operators occur in the course of the computation.

An alternate approach by Carruthers and Nieto [16] proceeds by defining new operators that correspond to sin $\hat{\theta}$ and cos $\hat{\theta}$, and derive their appropriate commutation relations. This avoids the above problems since one never deals with $\hat{\theta}$ itself, and the periodicity of these operators is guaranteed by construction. Unfortunately, in the examples given in the introduction, we are often interested in $\dot{\hat{\theta}} = [\hat{\theta}, H]/\mathrm{i}\hbar$, so the question at hand cannot be avoided in this manner.

Susskind and Glogower [14] introduce a generalized periodic phase operator which we shall call $\hat{\Phi}_{\mathrm{SG}}$, to avoid confusion. It is the periodic extension of $\hat{\theta}$, a sawtooth wave defined by: $\hat{\Phi}_{\mathrm{SG}}(\hat{\theta}) = [(\hat{\theta} + \pi) \bmod 2\pi] - \pi$. This new operator has the commutation relation

$$[\hat{L}, \hat{\Phi}_{\mathrm{SG}}] = \mathrm{i}(1 - 2\pi\delta(\hat{\Phi}_{\mathrm{SG}} - \pi)). \tag{9}$$

Yet another approach is that of Barnett and Pegg [17] who derive a representation for the phase operator $\hat{\Phi}_{\mathrm{BP}}$ when the number of angular momentum states is finite, $-l_0 \leqslant m \leqslant l_0$. The commutation relations are calculated for fixed l_0, and then the limit $l_0 \to \infty$ should only be taken at the end of the calculations [17]. They obtain

$$[\hat{L}, \hat{\Phi}_{\mathrm{BP}}] = \frac{-2\pi\hbar}{2l+1} \sum_{\substack{m,m'=-l_0 \\ m \neq m'}}^{l_0} \frac{(m-m')}{\exp[2\pi\mathrm{i}(m-m')(2l-1)]-1} |m'\rangle\langle m|. \tag{10}$$

Equation (9) can be obtained as a special case of (10), as discussed in [17]. Note that in both cases (9) and (10) the commutator is not a simple *c*-number, as it is in (1). This has drastic consequences for the calculation of many dynamical quantities, in atomic, optical and solid state physics. To the best of our knowledge, no physical consequences of the operator character of these commutation relations have been calculated theoretically or observed experimentally.

It is worth noting that the above candidates (9) and (10) for replacing the standard commutation relation predict that the angular momentum of a free particle is not simply related to its angular velocity. One might expect that for large enough rings and values of the angular momentum, one would obtain an Ehrenfest-like result, so that $\dot{\theta} \propto L$. However, given the free particle Hamiltonian for a bead of mass m on a circle of radius R,

$$H = \frac{\hat{L}^2}{2mR^2} \tag{11}$$

one finds using (9) or (10),

$$\langle n|\dot{\hat{\Phi}}|n\rangle = \frac{1}{\mathrm{i}\hbar}\langle n|[\hat{\Phi}, H]|n\rangle = \frac{-\mathrm{i}}{2mR^2}\langle n|\hat{L}[\hat{\Phi}, \hat{L}] + [\hat{\Phi}, \hat{L}]\hat{L}|n\rangle = 0. \tag{12}$$

We see that the expectation value of the angular velocity in any eigenstate of the angular momentum is identically zero. Thus $\dot{\hat{\Phi}}$ does not have the usual meaning of an angular velocity in the classical limit, and thus loses connection with our standard physical interpretation. On the other hand, the commutation relation of (1) gives the desired result that $\langle n|\dot{\hat{\theta}}|n\rangle = n\hbar/mR^2$.

We emphasize that we do not claim that $\hat{\theta}$ is an observable, nor do we comment on the Heisenberg uncertainty relation for $\hat{\theta}$ and $\hat{L}$. These issues are separate from the question of the proper commutation relation, treated here. Alternative formulations of the phase operator may be useful in this context [16, 17]. We also do not deal with cases where the discrete operator (i.e. the 'momentum') takes on only non-negative integral values, such as the energy of a harmonic oscillator.

In summary, one must be careful when using phase operators in periodic quantum mechanical systems, especially with regard to questions of self-adjointness. We find that the standard definitions of phase and angular momentum operators lead to the standard commutation relations given in (1), and not to the inconsistent result claimed in the literature. In addition the standard approach gives results that correspond to what we expect of phase and angular momentum variables in the classical limit.

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